## **Supporting information**

# Charge, Adsorption, Water Stability and Bandgap Tuning of An Anionic Cd(II) Porphyrinic Metal-Organic Framework

Qi Li,<sup>a</sup> Yanping Luo,<sup>ad</sup> Yue Ding,<sup>a</sup> Yina Wang,<sup>a</sup> Yuxin Wang,<sup>a</sup> Hongbin Du,<sup>b</sup> Rongxin Yuan,<sup>c</sup> Jianchun Bao,<sup>d</sup> Min Fang,<sup>\*ab</sup> Yong Wu<sup>\*a</sup>

- <sup>a.</sup> Jiangsu Key Laboratory of New Power Batteries, Jiangsu Collaborative Innovation Center of Biomedical Functional Materials, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing 210023, PR China. Email: <u>fangmin@njnu.edu.cn</u>, wuyong@njnu.edu.cn
- <sup>b.</sup> State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, China
- <sup>c.</sup> School of Chemistry and Materials Engineering, Changshu Institute of Technology, Changshu, 215500, China.
- <sup>d.</sup> Jiansu Key Laboratory of Biofunctional Materials, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing 210023, China.

\* Corresponding authors.

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Compound	1	1(6:1)-2d
Formula	$C_{114.20}H_{98.80}Cd_{3.20}N_{14.60}$	$C_{113.76}H_{104.04}Cd_{3.31}N_{14.38}$
	O <sub>23.50</sub>	O <sub>24</sub>
Fw	1933.17	2408.47
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	C2/c
<i>a</i> (Å)	7.089(2)	7.0923 (16)
$b(\text{\AA})$	26.513(8)	26.431(6)
<i>c</i> (Å)	30.078(8)	30.165(8)
$\beta(^{\circ})$	95.351(8)	95.216(3)
$V(Å^3)$	5628(3)	5631(2)
Ζ	2	2
$D_e(g/cm^3)$	1.423	1.420
$\mu(mm^{-1})$	0.675	0.695
<i>T</i> (K)	296(2)	296(2)
Total reflections	32793	56916
Unique data collected	4906	6167
Observed reflections	3749	3210
$R_{\rm int}$	0.063	0.142
$R_1$ , $wR_2$ ( $I > 2\sigma(I)$ )	0.0951, 0.2695	0.086,0.1761
R <sub>1</sub> , wR <sub>2</sub> (all data)	0.1075, 0.2837	0.1671,0.2151
Goodness of fit on $F^2$	1.141	1.036

## Table S1 Crystallographic data for 1 and 1(6:1)-2d.

### Table S2 Selected bond distances (Å) and angles (degrees) for 1.

<u>C1-02</u>	1.24(2)	C13-C14	1.467(9)
C101	1.293(16)	C1—C2	1.497(18)
C14—C15	1.3900	C14—C19	1.3900
C2-C3	1 3900	C15-C16	1 3900
C2—C7	1.3900	C15—H15	0.9300
C3—C4	1.3900	C16—C17	1.3900
С3—НЗА	0.9599	C16—H16	0.9300
C4—C5	1 3900	C17—C18	1 3900
C4—H4A	0.9600	C17 - C20	1 561(11)
C5—C6	1 3900	C18-C19	1 3900
C5—C8	1 477(10)	C18—H18	0.9300
C6—C7	1.3900	C19—H19	0.9300
С6—Н6А	0.9601	C7—H7A	0.9600
O1—Cd2ii	2.314(8)	O1—Cd2iii	2.355(8)
O1—Cd1i	2.570(14)	O2—Cd1i	2.234(18)
C8—C24iv	1.339(12)	C8—C9	1.411(11)
C20—O4	1.247(9)	C20—O3	1.250(8)
C21—N2	1.372(9)	C21—C22	1.421(12)
C22—C23	1.343(16)	C22—H22A	0.9300
C23—C24	1.439(11)	С23—Н23А	0.9300
C24—N2	1.343(10)	Cd104	2.424(7)
Cd1—O4v	2.424(7)	Cd1—O3	2.521(13)
Cd1—O3v	2.521(13)	Cd2—Cd2vi	0.598(2)
C9—N1	1.373(11)	Cd2—O4vi	2.190(7)
C9—C10	1.480(13)	Cd2—O4	2.559(6)
C10-C11	1.326(15)	N2—H2A	0.8600
C10—H10A	0.9300	C11—C12	1.417(13)
C11—H11A	0.9300	C12—N1	1.365(9)
C12—C13	1.398(12)	C13—C21	1.400(13)
02C1O1	124.1(17)	O2—C1—C2	116.6(12)
O1—C1—C2	119.3(16)	O2—C1—Cd1i	54.4(10)
O1—C1—Cd1i	69.8(9)	C2-C1-Cd1i	170.3(11)
С3—С2—С7	120.0	C3—C2—C1	120.1(9)
C7—C2—C1	119.8(9)	C4—C3—C2	120.0
С4—С3—НЗА	120.0	O4—C20—O3	121.8(6)
С2—С3—НЗА	120.0	C3—C4—C5	120.0
C3—C4—H4A	120.0	O4—C20—C17	120.1(5)
C5—C4—H4A	120.0	O3—C20—C17	117.7(6)
C6—C5—C4	120.0	C6—C5—C8	121.9(6)
C4—C5—C8	118.1(6)	C5—C6—C7	120.0
N2-C21-C13	127.7(6)	С5—С6—Н6А	120.0
N2-C21-C22	107.3(9)	С7—С6—Н6А	120.0
C13—C21—C22	125.0(7)	C6—C7—C2	120.0
C23—C22—C21	107.5(7)	С6—С7—Н7А	120.0
С23—С22—Н22А	126.3	С2—С7—Н7А	120.0
C21—C22—H22A	126.3	C1-O1-Cd2ii	134.2(8)
C22—C23—C24	108.5(9)	C1-O1-Cd2iii	141.2(8)
С22—С23—Н23А	125.7	Cd2ii—O1—Cd2iii	14.69(8)
C24—C23—H23A	125.7	C1—O1—Cd1i	82.1(11)
C8iv—C24—N2	125.9(7)	Cd2ii—O1—Cd1i	91.1(4)
C8iv-C24-C23	127.4(9)	Cd2iii—O1—Cd1i	104.3(4)
N2-C24-C23	106.6(8)	C1—O2—Cd1i	98.7(10)
O2vii—Cd1—O2i	77.5(10)	C24iv—C8—C9	128.6(8)
O2vii—Cd1—O4	125.0(5)	O2i-Cd1-O4	86.0(5)
C24iv—C8—C5	111.1(7)	O2vii—Cd1—O4v	86.0(4)
C9—C8—C5	120.2(9)	O4—Cd1—O4v	142.2(8)
O2i—Cd1—O4v	125.0(5)	O2i—Cd1—O3	96.5(4)

O2vii—Cd1—O3	173.9(7)	O2vii—Cd1—O1i	84.9(6)
O4—Cd1—O3	52.3(3)	O2i—Cd1—O1i	54.9(5)
C19—C14—C13	116.7(6)	C20—O4—Cd2	153.8(5)
C14-C15-C16	120.0	Cd2vi—O4—Cd2	11.43(6)
C14-C15-H15	120.0	Cd1	102.7(4)
C16-C15-H15	120.0	C17-C16-C15	120.0
C17-C16-H16	120.0	C15-C16-H16	120.0
C18—C17—C16	120.0	C18-C17-C20	117.7(5)
C16—C17—C20	121.7(5)	C19-C18-C17	120.0
C19-C18-H18	120.0	C17-C18-H18	120.0
C18-C19-C14	120.0	C18-C19-H19	120.0
C14-C19-H19	120.0	O2-C1-C2-C3	-10.0(16)
C21—C13—C14—C19	-76.8(9)	C17—C20—O4—Cd2	-44.1(19)
O1—C1—C2—C3	169.9(9)	C19-C14-C15-C16	0.0
O2—C1—C2—C7	167.5(11)	C13-C14-C15-C16	169.7(11)
01—C1—C2—C7	-12.6(14)	C14-C15-C16-C17	0.0
C7—C2—C3—C4	0.0	C15-C16-C17-C18	0.0
C1—C2—C3—C4	177.5(9)	C15-C16-C17-C20	-171.0(10)
C2—C3—C4—C5	0.0	C16-C17-C18-C19	0.0
C3—C4—C5—C6	0.0	C20-C17-C18-C19	171.4(10)
C3—C4—C5—C8	179.0(8)	C17—C18—C19—C14	0.0
C4—C5—C6—C7	0.0	C15-C14-C19-C18	0.0
C8—C5—C6—C7	-178.9(9)	C13-C14-C19-C18	-170.3(11)
C5—C6—C7—C2	0.0	C3—C2—C7—C6	0.0
C1—C2—C7—C6	-177.5(9)	C12—C13—C14'—C19'	98.3(13)
02—C1—O1—Cd2ii	87.5(19)	C2-C1-O1-Cd2ii	-92.4(17)
Cd1i-C1-O1-Cd2ii	83.8(13)	02-C1-01-Cd2iii	106.8(19)
C2-C1-O1-Cd2iii	-73(2)	Cd1i—C1—O1—Cd2iii	103.0(16)
02-C1-O1-Cd1i	3.8(15)	C2-C1-O1-Cd1i	-176.1(11)
01-C1-02-Cd1i	-4.3(17)	C2-C1-O2-Cd1i	175.6(9)
C6-C5-C8-C24iv	57.8(9)	C4—C5—C8—C24iv	-121.2(7)
C6—C5—C8—C9	-118.1(9)	C4—C5—C8—C9	62.9(10)
C18—C17—C20—O4	2.1(13)	C17—C20—O4	173.3(7)
C18-C17-C20-O3	174.8(8)	C17—C20—O3	-14.0(12)
C13-C21-N2	1.9(12)	C14—C13—C21—N2	178.1(7)
C13—C21—N2	166.2(12)	C12-C13-C21-C22	-1792(8)
C13 - C21 - C22	-30(11)	C13-C21-C22	-149(15)
$N_{2}$ C21 C22 C23	-0.4(10)	$C_{21} - C_{22} - C_{23}$	-179 5(8)
$C_{21} - C_{22} - C_{23} - C_{24}$	0 4(10)	C22 - C23 - C24 - C8iv	-1762(9)
$C_{22}$ $C_{23}$ $C_{24}$ $N_{2}$	-0.2(10)	C13-C12-N1-C9	175 9(7)
C11-C12-N1-C9	-2.7(9)	C8 - C9 - N1 - C12	-175.6
C24iv - C8 - C9 - N1	-1.6(14)	C10-C9-N1-C12	4 5(10)
$C_{5}$ $C_{8}$ $C_{9}$ $N_{1}$	173 5(8)	C8iv - C24 - N2 - C21	176.0(7)
$C_{24iv} = C_{8} = C_{9} = C_{10}$	178 3(10)	$C_{23}$ $C_{24}$ $N_{2}$ $C_{21}$ $C_{21}$	-0.1(8)
$C_{2-1}^{-1} = C_{2-1}^{-1} = C_{2$	-6.6(14)	$C_{23} = C_{24} = N_2 = C_{24}$	179 4(7)
$C_{22}$ $C_{21}$ $N_{2}$ $C_{24}$	0.3(8)	N1_C9_C10_C11	-4 6(12)
$C_{22} = C_{21} = 10 = C_{11}$	0.5(8)	$04 - C^{20} - 03 - C^{41}$	-11.3(10)
$C_0 - C_1 $	2 9(13)	$C_17 - C_20 - O_3 - C_{41}$	176 1(9)
$C_{10} = C_{10} = C_{11} = C_{12}$	-0.2(13)	$C_{11} = C_{20} = 0_{3} = C_{01}$	-178 8(0)
N1 - C12 - C12 - C12	1.2(13)	03 - 020 = 04 = 042	174.6(8)
111 - 012 - 013 - 021	1.3(12) 170 6(0)	$C_{17} C_{20} - C_{4} - C_{4$	-62.0(15)
11 - 012 - 013 - 021	-174.4(8)	$C_1 = C_2 = 04 = C_4 =$	52.9(13)
11 - 012 - 013 - 014	1/4.4(0) 2 Q(12)	$C_{17}$ $C_{20}$ $C_{4}$ $C_{41}$	-175.7(10)
C12 - C12 - C13 - C14	-70.6(11)	$C_{1} = C_{20} = 04 = C_{01}$	1/3.7(10)
$C_{12}$ $-C_{13}$ $-C_{14}$ $-C_{13}$	142 4(0)	$C_{12} = C_{13} = C_{14} = C_{15}$	113.2(7)
03-020-04-042	143.4(7)		

Symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x, -y+1, -z+1; (iii) x-1, -y+1, z-1/2; (iv) -x-1/2, -y+1/2, -z+1; (v) -x+2, y, -z+3/2; (vi) -x+1, y, -z+3/2; (vii) x+1, -y+1, z+1/2.

## Table S3 Selected bond distances (Å) and angles (degrees) for 1(6:1)-2d.

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		ances	A) and angles (d			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Cd1—O2	2.344	(5)	C21B—C20B	1.41	(2)
	Cd1—O2i	2.344	(5)	C13B—C14B	1.45	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Cd1—O1i	2 3 5 3	) (6)	C18B—C17B	1.51	$\tilde{\alpha}$
$ \begin{array}{c} \mathrm{Cd} & -0.5 \mathrm{in} & -2.4 \mathrm{Q} & (1) & \mathrm{Cd} & -0.5 \mathrm{R} & 0.930 \\ \mathrm{Cd} & -0.5 \mathrm{in} & 2.4 \mathrm{Q} & (1) & \mathrm{Cd} & -0.5 \mathrm{R} & 0.930 \\ \mathrm{Cd} & -0.5 \mathrm{in} & 2.1 \mathrm{P} & (1) & \mathrm{Cd} & -0.5 \mathrm{A} & 1.23 \mathrm{R} & (18) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.1 \mathrm{P} & (19) & 0.4 - \mathrm{Cd} & 1.6 \mathrm{A} & 1.6 \mathrm{A} & (16) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{P} & (6) & \mathrm{N2} - \mathrm{Cl} \mathrm{A} & 1.6 \mathrm{A} & (16) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{P} & (6) & \mathrm{N2} - \mathrm{Cl} \mathrm{A} & 1.6 \mathrm{A} & (16) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{H} & (4) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{H} & (4) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.5 \mathrm{I} & (18) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{Q} & (4) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{Q} & (4) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 2.3 \mathrm{Q} & (8) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{Q} & (4) \\ \mathrm{Cd} & -0.5 \mathrm{Ai} & 1.3 \mathrm{Q} & (10) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{Q} & (4) \\ \mathrm{Cd} - 0.5 \mathrm{Ai} & 1.4 \mathrm{Q} & (12) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{Q} & (6) \\ \mathrm{Cl} - \mathrm{Cl} & 1.2 \mathrm{S} & (9) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & (4) \\ \mathrm{Cl} - \mathrm{Cl} & 1.3 \mathrm{S} & (10) & \mathrm{Cl} \mathrm{A} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & (4) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 1.4 \mathrm{Q} & (12) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & (4) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 1.4 \mathrm{Q} & (12) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & 1.5 \mathrm{I} & (2) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 1.5 \mathrm{I} & (2) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & 0 & (6) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 0 & (6) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & 0 & (6) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 0 & (6) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.4 \mathrm{A} & 0 & (6) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 1.5 \mathrm{I} & (2) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.3 \mathrm{A} & (1) \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 0 & (6) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.3 \mathrm{A} & 0 \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 0 & (6) & \mathrm{Cl} - \mathrm{Cl} \mathrm{A} & 1.3 \mathrm{A} & 0 \\ \mathrm{Cl} - \mathrm{Cl} - \mathrm{Cl} & 1.4 \mathrm{A} & 0 & 0.3 \mathrm{O} & \mathrm{Cl} & \mathrm{Cl} + \mathrm{Cl} + $		2.555	(0)	C14D U14D	0.020	(2)
$ \begin{array}{c} \mathrm{cd} - 0.3 \mathrm{dh} & 2.402 & (11) & C2 \mathrm{dh} - 1.2 \mathrm{dh} & 0.9 \mathrm{dh} \\ \mathrm{cd} - 0.3 \mathrm{dh} & 2.117 & (19) & 0.4 - C3 \mathrm{A} & 1.238 & (18) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.157 & (10) & 0.4 - C3 \mathrm{A} & 1.238 & (18) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.357 & (10) & 0.4 - C3 \mathrm{A} & 1.63 & (19) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.357 & (10) & 0.4 - C3 \mathrm{A} & 1.63 & (19) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.357 & (10) & 0.4 - C3 \mathrm{A} & 1.64 & (17) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.340 & (8) & C1 \mathrm{A} - C1 \mathrm{A} & 1.40 & (7) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.340 & (8) & C1 \mathrm{A} - C2 \mathrm{A} & 1.515 & (18) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.438 & (18) & C1 \mathrm{A} - C2 \mathrm{A} & 1.515 & (18) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.438 & (18) & C1 \mathrm{A} - C1 \mathrm{A} & 1.44 & (1) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.438 & (18) & C1 \mathrm{A} - C1 \mathrm{A} & 1.44 & (1) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.438 & (18) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.44 & (1) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 2.438 & (10) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.44 & (1) \\ \mathrm{cd} - 0.3 \mathrm{ch} & 1.238 & (10) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.44 & (1) \\ \mathrm{cd} - 0.1 & 1.234 & (8) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.45 & (1) \\ \mathrm{cd} - 0.1 & 1.368 & (10) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.44 & (1) \\ \mathrm{cd} - 0.1 & 1.368 & (10) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.51 & 0.9 \\ \mathrm{cd} - 0.1 & 1.368 & (13) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.51 & 0.9 \\ \mathrm{cd} - 0.1 & 1.362 & (13) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.51 & 0.2 \\ \mathrm{cd} - 0.1 & 1.362 & (13) & C1 \mathrm{A} - C1 \mathrm{SA} & 1.51 & 0.2 \\ \mathrm{cd} - 0.23 & 1.23 \mathrm{A} & 1.36 & (11) & C3 \mathrm{A} - C1 \mathrm{SA} & 1.38 & (1) \\ \mathrm{cd} - C2 \mathrm{S} & 1.380 & (11) & C3 \mathrm{A} - C1 \mathrm{SA} & 1.38 & (1) \\ \mathrm{cd} - C3 \mathrm{S} & 1.380 & (11) & C3 \mathrm{A} - C1 \mathrm{SA} & 1.38 & (1) \\ \mathrm{cd} - C3 \mathrm{S} & 1.380 & (11) & C3 \mathrm{A} - C1 \mathrm{A} & 1.390 \\ \mathrm{cd} - C2 \mathrm{R} & 1.28 & (2) & C2 \mathrm{A} - C1 \mathrm{A} & 1.38 & (3) \\ \mathrm{cd} - C2 \mathrm{R} & 1.28 & (12) & C1 \mathrm{B} - C1 \mathrm{B} & 1.390 \\ \mathrm{cd} - C2 \mathrm{R} & 1.28 & (12) & C1 \mathrm{B} - C1 \mathrm{B} & 1.390 \\ \mathrm{cd} - C1 \mathrm{A} & 1.48 & (3) & C3 \mathrm{CB} - C4 \mathrm{B} & 1.390 \\ \mathrm{cd} - C2 \mathrm{A} & 1.38 & (3) & C3 \mathrm{CB} - C4 \mathrm{B} & 1.390 \\ \mathrm{cd} - C1 \mathrm{A} & 1.48 & (3) & C3 \mathrm{CB} - C4 \mathrm{A} & 1.300 \\ \mathrm{cd} - C2 \mathrm{R} & 1.333 & (13) & C3 - C4 \mathrm{A} & 1.300 \\ \mathrm{cd} - C1 \mathrm{B} & 1.333 &$		2.333	(0)	С14В—н14В	0.930	
$ \begin{array}{c} \mathrm{Cd} - 0.35 \mathrm{lin} & 2.402 & (11) & \mathrm{C20B} - 1208 & 0.930 \\ \mathrm{Cd} - 0.4\mathrm{Ain} & 2.117 & (19) & 0.3\mathrm{A} - C24\mathrm{A} & 1.228 & (18) \\ \mathrm{Cd} - 0.4\mathrm{Ain} & 2.117 & (19) & 0.3\mathrm{A} - C24\mathrm{A} & 1.242 & (18) \\ \mathrm{Cd} - 0.4\mathrm{Ain} & 2.117 & (19) & 0.3\mathrm{A} - C13\mathrm{A} & 1.31 & (7) \\ \mathrm{Cd} - 0.27 & 2.375 & (6) & N2\mathrm{A} - C13\mathrm{A} & 1.44 & (7) \\ \mathrm{Cd} - 0.4\mathrm{Nin} & 2.340 & (8) & C13\mathrm{A} - C13\mathrm{A} & 1.44 & (7) \\ \mathrm{Cd} - 0.4\mathrm{Nin} & 2.340 & (8) & C13\mathrm{A} - C13\mathrm{A} & 1.44 & (7) \\ \mathrm{Cd} - 0.4\mathrm{Nin} & 2.340 & (8) & C13\mathrm{A} - C13\mathrm{A} & 1.44 & (7) \\ \mathrm{Cd} - 0.4\mathrm{Nin} & 2.348 & (8) & C14\mathrm{A} - C15\mathrm{A} & 1.45 & (19) \\ \mathrm{Cd} - 0.4\mathrm{Nin} & 2.348 & (8) & C14\mathrm{A} - C15\mathrm{A} & 1.45 & (6) \\ \mathrm{Cd} - 0.4\mathrm{A} & 1.245 & (9) & C14\mathrm{A} - H14\mathrm{A} & 0.920 \\ \mathrm{Cl} - 0.1 & 1.245 & (9) & C19\mathrm{A} - C18\mathrm{A} & 1.43 & (4) \\ \mathrm{Cl} - 0.1 & 1.245 & (19) & C19\mathrm{A} - C28\mathrm{A} & 1.38 & (4) \\ \mathrm{Cl} - C12\mathrm{I} & 1.355 & (10) & C19\mathrm{A} - C28\mathrm{A} & 1.38 & (4) \\ \mathrm{Cl} - C12\mathrm{I} & 1.450 & (12) & C22\mathrm{A} - H22\mathrm{A} & 0.930 \\ \mathrm{Cl} - C12\mathrm{-C178\mathrm{i} & 1.462 & (19) & C22\mathrm{A} - C23\mathrm{A} & 1.38 & (4) \\ \mathrm{Cl} - C12\mathrm{-C178\mathrm{i} & 1.462 & (19) & C22\mathrm{A} - C23\mathrm{A} & 1.35 & (4) \\ \mathrm{Cl} - C11\mathrm{I} & 0.930 & C15\mathrm{A} - C16\mathrm{A} & 1.51 & (2) \\ \mathrm{Cl}C11\mathrm{I} & 1.362 & (13) & C17\mathrm{A} - C18\mathrm{A} & 1.51 & (2) \\ \mathrm{Cl}C11\mathrm{I} & 0.930 & C15\mathrm{A} - C16\mathrm{A} & 1.51 & (2) \\ \mathrm{Cl}C13\mathrm{I} & 1.362 & (13) & C17\mathrm{A} - C18\mathrm{A} & 1.51 & (2) \\ \mathrm{Cl}C13\mathrm{I} & 1.58 & (3) & C2\mathrm{B} - C7\mathrm{B} & 1.390 \\ \mathrm{Cl} - C2\mathrm{A} & 1.48 & (12) & C17\mathrm{A} - C18\mathrm{A} & 1.51 & (2) \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (12) & C10\mathrm{-C18\mathrm{A} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (12) & C10\mathrm{-C18\mathrm{A} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (12) & C10\mathrm{-C18\mathrm{A} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (13) & C3\mathrm{-C48\mathrm{B} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (12) & C10\mathrm{-C18\mathrm{A} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (13) & C3\mathrm{-C48\mathrm{B} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (13) & C3\mathrm{-C48\mathrm{B} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & (13) & C3\mathrm{-C48\mathrm{H} & 1.390 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & 0.930 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & 0.930 \\ \mathrm{Cl}C2\mathrm{A} & 1.48 & 0.930$	Cd1—O3B11	2.402	(11)	C22B—H22B	0.930	
$ \begin{array}{c} \mathrm{Cd} -\mathrm{OAA} \mathrm{ini} & 2.117 & (19) & \mathrm{OAA} - C24A & 1.28 & (18) \\ \mathrm{Cd} -\mathrm{OAA} & 1.262 & (18) \\ \mathrm{Cd} -\mathrm{O2A} & 2.375 & (6) & \mathrm{N2A} - C13A & 1.31 & (7) \\ \mathrm{Cd} -\mathrm{O4B} & 2.340 & (8) & \mathrm{C13A} - C16A & 1.63 & (9) \\ \mathrm{Cd} -\mathrm{O4B} & 2.340 & (8) & \mathrm{C13A} - C1AA & 1.40 & (7) \\ \mathrm{Cd} -\mathrm{O4B} & 2.340 & (8) & \mathrm{C13A} - C1AA & 1.40 & (7) \\ \mathrm{Cd} -\mathrm{O3A} & 2.48 & (18) & \mathrm{C1A} - C2AA & 1.41 & (4) \\ \mathrm{Cd} -\mathrm{O3A} & 2.48 & (18) & \mathrm{C1A} - C2AA & 1.42 & (4) \\ \mathrm{Cd} -\mathrm{O3A} & 2.48 & (18) & \mathrm{C1A} - C1AA & 1.40 & (5) \\ \mathrm{Cd} -\mathrm{O4A} & 2.48 & (18) & \mathrm{C1A} - C1AA & 1.44 & (4) \\ \mathrm{Cd} -\mathrm{O3A} & 2.48 & (18) & \mathrm{C1A} - C1AA & 1.44 & (4) \\ \mathrm{Cd} -\mathrm{C1} & 1.245 & (9) & \mathrm{C1A} - C1AA & 1.44 & (6) \\ \mathrm{Cd} -\mathrm{C1} & 1.245 & (9) & \mathrm{C1A} - C1AA & 1.43 & 0.930 \\ \mathrm{C1} -\mathrm{C1} & 1.245 & (9) & \mathrm{C1A} - C1AA & 1.44 & (16) \\ \mathrm{C1} -\mathrm{C1} & 1.245 & (9) & \mathrm{C1A} - C1AA & 1.45 & (6) \\ \mathrm{C1} -\mathrm{C1} & 1.245 & (19) & \mathrm{C1A} - C1AA & 1.45 & (6) \\ \mathrm{C1} -\mathrm{C1} & 1.450 & (12) & \mathrm{C2A} - C2AA & 1.38 & (4) \\ \mathrm{C1} -\mathrm{C1} & 1.450 & (12) & \mathrm{C1A} - C1AA & 1.44 & (5) \\ \mathrm{C1} -\mathrm{C1} & 1.450 & (13) & \mathrm{C1A} - C1AA & 1.44 & (5) \\ \mathrm{C1} -\mathrm{C1} & 1.362 & (13) & \mathrm{C1A} - C1AA & 1.44 & (5) \\ \mathrm{C1} -\mathrm{C1} & 1.362 & (13) & \mathrm{C1A} - C1AA & 1.44 & (5) \\ \mathrm{C1} -\mathrm{C1} & 1.362 & (13) & \mathrm{C1A} - C1AA & 1.44 & (5) \\ \mathrm{C1} -\mathrm{C1} +\mathrm{I1} & 0.930 & \mathrm{C1A} - C1AA & 1.48 & (4) \\ \mathrm{C2} - C13B & 1.28 & (2) & \mathrm{C2} - C1B & 1.38 & (4) \\ \mathrm{C2} - C13B & 1.28 & (2) & \mathrm{C2} - C1B & 1.38 & (4) \\ \mathrm{C2} - C13B & 1.28 & (2) & \mathrm{C2} - C1B & 1.390 \\ \mathrm{C1} - C2B & 1.38 & (3) & \mathrm{C2} - C1B & 1.390 \\ \mathrm{C1} - C2B & 1.38 & 1.316 & (3) & \mathrm{C3} - C4B & 1.390 \\ \mathrm{C1} - C2B & 1.38 & 1.316 & (3) & \mathrm{C3} - C4B & 1.390 \\ \mathrm{C1} - C2B & 1.376 & (18) & \mathrm{C3} - C4A & 1.390 \\ \mathrm{C1} - C4B & 1.390 \\ \mathrm{C1} - C4B & 1.376 & (18) & \mathrm{C3} - C4A & 1.390 \\ \mathrm{C1} - C4B & 1.390 & \mathrm{C1} - C4A & 1.390 \\ \mathrm{C1} - C4B & 1.390 & \mathrm{C2} - C4A & 1.390 \\ \mathrm{C1} - C4B & 1.390 & \mathrm{C2} - C4A & 1.390 \\ \mathrm{C1} - C4B & 1.390 & \mathrm{C2} - C4A & 1.390 \\ \mathrm{C1} - C4B - C1B & 1.376 & (18) & \mathrm{C3} - C4A & 1.390 \\ \mathrm{C1} - C1B & 1.31$	Cd1—O3Biii	2.402	(11)	C20B—H20B	0.930	
$ \begin{array}{c} \mbox{cd} = 0 cd$	Cd1 = O4Aiii	2 1 1 7	(19)	$O_{1}A = C_{2}A$	1 238	(18)
$ \begin{array}{c} \mathrm{Cd} -\mathrm{Cd} +\mathrm{Cd} +\mathrm$		2.117	(19)	014 024	1.250	(18)
$\begin{array}{c} \mathrm{Cd} D-\mathrm{Q} 2\nu & 2375 & (6) & \mathrm{NA}-\mathrm{ClA} & 131 & (7) \\ \mathrm{Cd} D-\mathrm{Q} 2\nu & 2375 & (6) & \mathrm{NA}-\mathrm{ClA} & 1.63 & (9) \\ \mathrm{Cd} D-\mathrm{Q} 2-\mathrm{Q} B\nu i & 2340 & (8) & \mathrm{ClA}-\mathrm{ClA} & 1.63 & (9) \\ \mathrm{Cd} D-\mathrm{Q} 2-\mathrm{Q} B\nu i & 2340 & (8) & \mathrm{ClA}-\mathrm{ClA} & 1.515 & (18) \\ \mathrm{Cd} D-\mathrm{Q} 2-\mathrm{Q} B\nu i & 2340 & (8) & \mathrm{ClA}-\mathrm{ClA} & 1.515 & (18) \\ \mathrm{Cd} D-\mathrm{Q} & 2.438 & (18) & \mathrm{ClA}-\mathrm{ClA} & 1.515 & (18) \\ \mathrm{Q} -\mathrm{Cl} & 2.438 & (18) & \mathrm{ClA}-\mathrm{ClA} & 1.515 & (16) \\ \mathrm{Q} -\mathrm{Cl} & 1.235 & (10) & \mathrm{ClA}-\mathrm{ClA} & 1.53 & (6) \\ \mathrm{Cl} -\mathrm{Cl} & 1.235 & (10) & \mathrm{ClA}-\mathrm{ClA} & 1.53 & (6) \\ \mathrm{Cl} -\mathrm{Cl} & 1.235 & (10) & \mathrm{ClA}-\mathrm{ClA} & 1.53 & (6) \\ \mathrm{Cl} -\mathrm{Cl} & 1.235 & (10) & \mathrm{ClA}-\mathrm{ClA} & 1.34 & (6) \\ \mathrm{Cl} -\mathrm{Cl} & 1.35 & (10) & \mathrm{ClA}-\mathrm{ClA} & 1.35 & (6) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.450 & (12) & \mathrm{ClA}-\mathrm{ClA} & 1.35 & (6) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.450 & (12) & \mathrm{ClA}-\mathrm{ClA} & 1.55 & (6) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.450 & (12) & \mathrm{ClA}-\mathrm{ClA} & 1.51 & (2) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.362 & (13) & \mathrm{ClA}-\mathrm{ClA} & 1.41 & (5) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.362 & (13) & \mathrm{ClA}-\mathrm{ClA} & 1.41 & (5) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.362 & (13) & \mathrm{ClA}-\mathrm{ClA} & 1.31 & (2) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.426 & (13) & \mathrm{ClA}-\mathrm{ClA} & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.426 & (13) & \mathrm{ClA}-\mathrm{ClA} & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.44 & (5) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.44 & (5) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.516 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.44 & (5) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.516 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.44 & (5) \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.516 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.518 & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.516 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.518 & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.516 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.518 & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.517 & (9) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.500 & 0.30 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.517 & (9) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.390 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.370 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.390 & 0 \\ \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} & 1.371 & (1) & \mathrm{Cl} -\mathrm{Cl} -\mathrm{Cl} -$	Cal—O4Aii	2.11/	(19)	03A—C24A	1.262	(18)
$\begin{array}{ccccc} {\rm Cd2-OdW} & 2375 & (6) & N2A-C16A & 1.63 & (9) \\ {\rm Cd2-OdW} & 2340 & (8) & C13A-C14A & 1.40 & (7) \\ {\rm Cd2-O3AW} & 2.438 & (18) & C1A-C2A & 1.44 & (4) \\ {\rm Cd2-O3AW} & 2.438 & (18) & C1A-C2A & 1.42 & (4) \\ {\rm Cd2-O3AW} & 2.438 & (18) & C1A-C1A & 1.42 & (4) \\ {\rm Cd2-O1AW} & 2.438 & (18) & C1A-C1A & 1.42 & (4) \\ {\rm Cd2-O1AW} & 2.438 & (18) & C1A-C1A & 1.43 & (6) \\ {\rm Cl-C1} & 1.234 & (8) & C1A-C1A & 1.43 & (6) \\ {\rm Cl-C1} & 1.235 & (10) & C19A-C1A & 1.43 & (4) \\ {\rm Cl-C1} & 1.245 & (9) & C1A-H1A & 0.930 & (4) \\ {\rm Cl-C1} & 1.245 & (9) & C1A-H1A & 0.930 & (4) \\ {\rm Cl-C1} & 1.245 & (12) & C2A-L12A & 0.930 & (4) \\ {\rm Cl-C1} & 1.456 & (12) & C2A-L12A & 0.930 & (6) \\ {\rm Cl-C1} & 1.456 & (12) & C2A-L12A & 0.930 & (6) \\ {\rm Cl-C-C1} & 1.456 & (12) & C2A-L12A & 0.930 & (6) \\ {\rm Cl-C-C1} & 1.456 & (13) & C17A-C16A & 1.41 & (5) \\ {\rm Cl-C-C1} & 1.456 & (13) & C17A-C16A & 1.41 & (5) \\ {\rm Cl-C-C1} & 1.456 & (13) & C17A-C16A & 1.41 & (5) \\ {\rm Cl-C-C1} & 1.456 & (13) & C17A-C16A & 1.43 & (6) \\ {\rm Cl-C1} & 1.456 & (13) & C17A-C16A & 1.41 & (5) \\ {\rm Cl-C-C3} & 1.458 & (3) & C18-C18 & 1.390 & (6) \\ {\rm Cl-C3} & 1.458 & (3) & C18-C18 & 1.390 & (6) \\ {\rm Cl-C3} & 1.458 & (3) & C18-C18 & 1.390 & (6) \\ {\rm Cl-C2} & 1.458 & (3) & C18-C18 & 1.390 & (6) \\ {\rm Cl-C2} & 1.458 & 1.280 & (2) & C20A-H20A & 0.930 & (7) \\ {\rm Cl-C2} & 1.451 & (9) & C28-C78 & 1.390 & (7) \\ {\rm Cl-C2} & 1.451 & (9) & C28-C78 & 1.390 & (7) \\ {\rm Cl-C2} & 1.517 & (9) & C28-C78 & 1.390 & (7) \\ {\rm Cl-C2} & 1.517 & (9) & C28-C78 & 1.390 & (7) \\ {\rm Cl-C2} & 1.517 & (9) & C28-C78 & 1.390 & (7) \\ {\rm Cl-C2} & 1.518 & 1.43 & (3) & C8-C48 & 1.390 & (7) \\ {\rm Cl-C2} & 1.518 & 1.37 & (2) & C8A-C4A & 1.390 & (7) \\ {\rm Cl-C4} & 1.518 & 1.37 & (2) & C3A-C43 & 1.390 & (2) \\ {\rm Cl-C1} & 1.518 & 1.37 & (2) & C3A-C4A & 1.390 & (2) \\ {\rm Cl-C1} & 1.518 & 1.37 & (2) & C3A-C4A & 1.390 & (2) & (2) & C3A-C4A & 1.390 & (2) & C3B-C18B-C19B & 10.41 & (1) & (1) & (2) & C2B-C19B & 10.41 & (1) & (2) & C2B-C19B & 10.41 & (1) & (2) & C2B-C10A & 1.38 & (3) & (2) & C2B-C18B-C19B & 10.41 & (1) &$	Cd2—O2iv	2.375	(6)	N2A—C13A	1.31	(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cd2—O2v	2.375	(6)	N2A—C16A	1.63	(9)
$ \begin{array}{c} \label{eq:constraints} & 2.30 & (9) & C1A-C2A & 1.44 & (1) \\ CdD-OJA, & 2.439 & (18) & C1A-C2A & 1.515 & (18) \\ CdD-OJA, & 2.439 & (18) & C1A-C2A & 1.42 & (4) \\ O2-C1 & 1.235 & (9) & C1A-C1A & 1.43 & (4) \\ OI-C1 & 1.234 & (8) & C1A-C1A & 1.43 & (6) \\ OI-C1 & 1.235 & (10) & C19A-C1BA & 1.43 & (4) \\ OI-C1 & 1.235 & (10) & C19A-C1AA & 1.43 & (4) \\ OI-C1 & 1.430 & (12) & C2A-C2A & 0.390 & (22-C1BK & 1.450 & (12) & C2A-C2A & 0.390 & (22-C1BK & 1.450 & (12) & C2A-C2A & 0.390 & (22-C1BK & 1.460 & (12) & C2A-C2A & 0.390 & (22-C1BK & 1.460 & (13) & C1A-C16A & 1.41 & (5) & (21-C1BK & 1.426 & (13) & C1A-C16A & 1.51 & (2) & (21-C1BK & 1.426 & (13) & C1A-C16A & 1.51 & (2) & (21-C1BK & 1.28 & (2) & C2A-C2A & 0.390 & (23-C1BK & 1.38 & (4) & (23-C1BK & 1.38 & (4) & (23-C1BK & 1.38 & (4) & (23-C1BA & 1.38 & (3) & (23-C1A & 1.39) & (23-C1BA & 1.38 & (3) & (23-C1BA & 1.39) & (23-C1BA & 1.38 & (3) & (23-C1BA & 1.38 & (3) & (23-C1BA & 1.38 & (3) & (23-C1BA & 1.39) & (23-$	$Cd^2 = OABvi$	2 3 4 0	$\binom{(2)}{(8)}$	C13A = C14A	1.40	(7)
$ \begin{array}{c} Cd_2 - 04801 & 2.440 & (3) & ClA - ClA & 1.44 & (4) \\ Cd_2 - 03A & 2.430 & (18) & ClA - ClA & 1.41A & 0.50 & 0 \\ Cd_2 - Cl & 1.451 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.451 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.451 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.455 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.555 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.555 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - Cl & 1.555 & (0) & ClA - ClA & 1.4A & 0.57 & 0 \\ Old - ClA & 1.4A & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0.57 & 0$	C12-04DVI	2.340	(8)		1.40	(r)
$\begin{array}{c} \mathrm{Cd} 2-03\mathrm{A}^{\mathrm{ini}} & 2.438 & (18) & \mathrm{C1} \mathrm{LA}-\mathrm{C2} \mathrm{A} & 1.515 & (18) \\ \mathrm{Cd} 2-\mathrm{C1} & 1.248 & (9) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{A} & 0.930 & \\ \mathrm{O1-C1} & 1.234 & (9) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{A} & 0.930 & \\ \mathrm{O1-C1} & 1.234 & (9) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{A} & 0.930 & \\ \mathrm{O1-C1} & 1.235 & (10) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.43 & (4) & \\ \mathrm{O1-C2} & 1.355 & (10) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.43 & (4) & \\ \mathrm{O1-C1} & 1.358 & (10) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.43 & (4) & \\ \mathrm{O1-C2} & 1.355 & (10) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.43 & (4) & \\ \mathrm{O1-C1} & 1.368 & (9) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.33 & (4) & \\ \mathrm{C1} \mathrm{C1}^{-1} \mathrm{C1} \mathrm{A} & 1.36 & (12) & \mathrm{C2} \mathrm{Z} \mathrm{A}-\mathrm{C2} \mathrm{A} & 1.35 & (12) & \\ \mathrm{C1} \mathrm{C1}^{-1} \mathrm{C1} \mathrm{A} & 1.27 & (4) & \mathrm{C1} \mathrm{S} \mathrm{A} & 1.15 & 0.930 & \\ \mathrm{C1} \mathrm{C1}^{-1} \mathrm{C1} \mathrm{A} & 1.262 & (13) & \mathrm{C1}^{-1} \mathrm{C1} \mathrm{S} \mathrm{A} & 1.15 & (2) & \\ \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{I} & 1.462 & (13) & \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & (2) & \\ \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{I} & 1.462 & (13) & \mathrm{C1} \mathrm{C1} \mathrm{A}-\mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & (2) & \\ \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{I} & 1.48 & (13) & \mathrm{C2} \mathrm{C2} \mathrm{C1} \mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & (2) & \\ \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{I} & 1.48 & (13) & \mathrm{C2} \mathrm{C2} \mathrm{C1} \mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & (2) & \\ \mathrm{C2} \mathrm{C1} \mathrm{C1} \mathrm{A} & 1.54 & (2) & \mathrm{C3} \mathrm{A} - \mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & \\ \mathrm{C2} \mathrm{C2} \mathrm{C1} \mathrm{A} & 1.54 & (2) & \mathrm{C3} \mathrm{C1} \mathrm{C1} \mathrm{S} \mathrm{A} & 1.51 & \\ \mathrm{C2} \mathrm{C2} \mathrm{C1} \mathrm{A} & 1.54 & (12) & \mathrm{C3} \mathrm{A} - \mathrm{C1} \mathrm{A} & 1.390 & \\ \mathrm{C3} \mathrm{C2} \mathrm{C2} \mathrm{C3} \mathrm{A} & 1.54 & (2) & \mathrm{C3} \mathrm{B} - \mathrm{C3} \mathrm{B} & 1.390 & \\ \mathrm{C4} \mathrm{C2} \mathrm{C2} \mathrm{A} & 1.54 & (3) & \mathrm{C3} \mathrm{B} - \mathrm{C3} \mathrm{B} & 1.390 & \\ \mathrm{C1} \mathrm{C2} \mathrm{C2} \mathrm{A} & 1.54 & (12) & \mathrm{C3} \mathrm{B} - \mathrm{C3} \mathrm{B} & 1.390 & \\ \mathrm{C1} \mathrm{C2} \mathrm{C2} \mathrm{A} & 1.37 & (9) & \mathrm{C3} \mathrm{C4} - \mathrm{C4} \mathrm{A} & 1.390 & \\ \mathrm{C1} \mathrm{C2} \mathrm{C2} \mathrm{A} & 1.37 & (1) & \mathrm{C3} \mathrm{C4} \mathrm{C4} \mathrm{A} & 1.390 & \\ \mathrm{C1} \mathrm{C2} \mathrm{C1} \mathrm{A} & 1.37 & (2) & \mathrm{C3} \mathrm{A} - \mathrm{C4} \mathrm{A} & 1.390 & \\ \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{C1} \mathrm{A} & 1.33 & (1) & \\ \mathrm{C2} \mathrm{C2} \mathrm{C1} \mathrm{A} & 1.33 & (1) & \\ \mathrm{C2} \mathrm{C1} \mathrm{C1} \mathrm{A} & 1.33 & (1) & \\ \mathrm{C2} C1$	Cd2—O4BVII	2.340	(8)	C21A—C22A	1.44	(4)
$\begin{array}{c} Cd2-C1 & 1.243 & (18) & C14-C10A & 1.42 & (4) \\ 02-C1 & 1.243 & (8) & C14A-C15A & 1.45 & (6) \\ NI-D1 & 0.860 & C19A-C18A & 1.43 & (4) \\ NI-C2 & 1.355 & (10) & C19A-C18A & 1.43 & (4) \\ NI-C2 & 1.355 & (10) & C19A-C18A & 1.43 & (4) \\ C12-C11 & 1.450 & (12) & C22A-C20A & 1.38 & (4) \\ C12-C17hix & 1.462 & (19) & C22A-C20A & 1.35 & (4) \\ C12-C17hix & 1.472 & (4) & C15A-L115A & 0.930 & \\ C12-C17hix & 1.450 & (19) & C22A-C16A & 1.40 & (6) \\ C10-C11 & 1.362 & (13) & C17A-C18A & 1.51 & (2) \\ C10-C11 & 1.362 & (13) & C17A-C18A & 1.51 & (2) \\ C10-C2 & 1.426 & (13) & C17A-C18A & 1.51 & (2) \\ C10-C11 & 1.362 & (13) & C17A-C18A & 1.51 & (2) \\ C10-C2 & 1.426 & (13) & C17A-C18A & 1.38 & (4) \\ C8-C13B & 1.28 & (2) & C20A-1120A & 0.930 & \\ C8-C13B & 1.28 & (2) & C20A-1120A & 0.930 & \\ C8-C3B & 1.496 & (9) & C3B-C2B & 1.390 & \\ C8-C5B & 1.496 & (11) & C3B-C18A & 1.38 & (4) \\ C8-C13B & 1.517 & (9) & C2B-C7B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 & \\ C1B-C17B & 1.27 & (4) & C6B-C5B & 1.390 & \\ C1B-C18B & 1.47 & (2) & C4B-H4B & 0.930 & \\ C1B-C18B & 1.47 & (2) & C3B-C18B & 1.390 & \\ C1B-C18B & 1.375 & (18) & C6A-16A & 0.930 & \\ C1B-C18B & 1.375 & (18) & C6A-16A & 0.930 & \\ C1B-C17B & 1.37 & (18) & C3B-C18B & \\ C1B-C17B & 1.33 & (19) & CA-C1A & 1.390 & \\ C1B-C18B & 1.33 & (19) & CA-C1A & 1.390 & \\ C1B-C18B & 1.33 & (19) & CA-C1A & 1.390 & \\ C1B-C1B & \\ C1B-C1B & 1.33 & (19) & C3B-C18B & \\ C1B-C1B &$	Cd2—O3Aviii	2.438	(18)	C21A—C24A	1.515	(18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cd2—O3A	2,439	(18)	C21A—C20A	1 42	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02 $C1$	1 245	(10)		0.020	(.)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		1.243	())		0.950	
$\begin{split} \mathbf{N}   -\mathbf{R}   \mathbf{N}   -\mathbf{C}   2 & \mathbf{C}   3 \\ \mathbf{N}   -\mathbf{C}   2 & 1 \\ 3 \\ \mathbf{N}   -\mathbf{C}   2 & 1 \\ 3 \\ \mathbf{C}   2 \\ \mathbf{C}   1 \\ \mathbf{C}   1 \\ \mathbf{C}   \mathbf{C} \\ \mathbf{C}   \mathbf{C}   \mathbf{C} \\ \mathbf{C} \\ \mathbf{C} \\ \mathbf{C}   \mathbf{C} \\ \mathbf{C} \\ \mathbf{C}   \mathbf{C} \\ \mathbf{C}   \mathbf{C} \\ \mathbf$	01-01	1.234	(8)	CI4A—CI5A	1.45	(6)
$\begin{split} \mathbf{N}   - \mathbb{C} ^2 &   1355 (10) & \mathbb{C} 9A - \mathbb{C} 8A &   1.43 (4) \\ \mathbb{C} 12 - \mathbb{C} 14 &   1.450 (12) & \mathbb{C} 22A - \mathbb{C} 22A &   0.390 \\ \mathbb{C} 12 - \mathbb{C} 17kix &   1.450 (12) & \mathbb{C} 22A - \mathbb{C} 22A &   0.390 \\ \mathbb{C} 12 - \mathbb{C} 17kix &   1.27 (4) & \mathbb{C} 15A - \mathbb{H} 15A &   0.390 \\ \mathbb{C} 10 - \mathbb{C} 11 &   0.930 & \mathbb{C} 15A - \mathbb{C} 6A &   1.40 (6) \\ \mathbb{C} 0 - \mathbb{C} 1 &   0.362 (13) & \mathbb{C} 17A - \mathbb{C} 6A &   1.41 (5) \\ \mathbb{C} 0 - \mathbb{C} 0 &   0.426 (13) & \mathbb{C} 17A - \mathbb{C} 6A &   1.41 (5) \\ \mathbb{C} 0 - \mathbb{C} 0 &   0.360 & (23A - \mathbb{H} 23A & 0.390 \\ \mathbb{C} -\mathbb{C} -\mathbb{C} 11 &   0.390 & \mathbb{C} 23A - \mathbb{H} 23A & 0.390 \\ \mathbb{C} -\mathbb{C} -\mathbb{C} 11 &   0.390 & (23A - \mathbb{H} 23A & 0.390 \\ \mathbb{C} -\mathbb{C} -\mathbb{C} 15A &   1.48 (6) & (23B - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2B &   1.517 (9) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2A &   1.517 (9) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2A &   1.517 (9) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2A &   1.48 (12) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2A &   1.45 (3) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2A &   1.45 (3) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2B &   1.47 (3) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2B &   1.47 (3) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} -\mathbb{C} 2B &   1.47 (3) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 16B - \mathbb{C} 18 &   1.47 (2) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 16B - \mathbb{C} 18 &   1.37 (2) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 16B - \mathbb{C} 18 &   1.37 (2) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 18 - \mathbb{C} 18 &   1.37 (2) & \mathbb{C} 18 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 18 - \mathbb{C} 18 &   1.39 &   1.91 & (3) & \mathbb{C} 14 - \mathbb{C} 13 &   1.390 \\ \mathbb{C} 18 - \mathbb{C} 18 &   1.39 &   1.91 & (3) & \mathbb{C} 14 - \mathbb{C} 18 &   1.390 \\ \mathbb{C} 18 - \mathbb{C} 2B &   1.39 &   1.91 &   1.39 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.39 &   1.91 &   1.39 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.39 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.39 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.38 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.38 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.38 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   1.39 &   1.11 &   1.19 \\ \mathbb{C} 2B - \mathbb{C} 2B &   $	N1—H1	0.860		C19A—H19A	0.930	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N1-C12	1.355	(10)	C19A—C18A	1.43	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1C9	1 368	(9)	C19A - C20A	1 38	(4)
$\begin{array}{c} C12-C17aix & 1.450 & (12) & C22A-H22A & 0.930 \\ C12-C17aix & 1.27 & (4) & C15A-H15A & 0.930 \\ C12-C17aix & 1.27 & (4) & C15A-H15A & 0.930 \\ C10-C11 & 1.362 & (13) & C17A-C16A & 1.40 & (6) \\ C10-C11 & 1.362 & (13) & C17A-C16A & 1.41 & (5) \\ C10-C12 & 1.426 & (13) & C17A-C16A & 1.41 & (5) \\ C1-C12 & 1.426 & (13) & C17A-C16A & 1.41 & (5) \\ C1-C14 & 0.930 & C23A-H23A & 0.930 \\ C23-C13B & 1.28 & (2) & C20A-H20A & 0.930 \\ C8-C13B & 1.28 & (2) & C20A-H20A & 0.930 \\ C8-C3B & 1.496 & (9) & C3B-C2B & 1.390 \\ C8-C3B & 1.517 & (9) & C2B-C7B & 1.390 \\ C1-C2B & 1.517 & (9) & C2B-C7B & 1.390 \\ C1-C2B & 1.517 & (9) & C2B-C7B & 1.390 \\ C1-C2A & 1.45 & (3) & C7B-C6B & 1.390 \\ C1-C2B & 1.517 & (9) & C2B-C7B & 1.390 \\ C1B-C24B & 1.228 & (12) & C7B-C6B & 1.390 \\ C1B-C24B & 1.228 & (14) & C6B-H6B & 0.930 \\ C1B-C24B & 1.227 & (4) & C6B-C5B & 1.390 \\ C16B-C15B & 1.47 & (2) & C4B-H4B & 0.930 \\ C16B-C15B & 1.47 & (2) & C4B-H4B & 0.930 \\ C16B-C17B & 1.37 & (3) & C5A-C6A & 1.390 \\ C19B-C18B & 1.326 & (3) & C7A-C7A & 1.390 \\ C19B-C18B & 1.326 & (3) & C7A-C7A & 1.390 \\ C18B-H19B & 0.930 & C7A-H7A & 0.930 \\ C18B-H19B & 0.930 & C7A-H7A & 0.930 \\ C18B-C18B & 1.326 & (3) & C7A-C2A & 1.390 \\ C2B-C2B & 1.38 & (18) \\ C2B-C4B & 0.53 & (12) & C3A-C4A & 1.390 \\ C1B-C4B & 0.53 & (13) & C1B-C14B-H14B & 1258 \\ O2-C41-O1 & 54.45 & (18) \\ O2-C41-O1 & 54.45 & (18) \\ O2-C41-O1 & 0.61 & (2) & C13B-C14B & 1187 & (13) \\ O2-C41-O1 & 0.61 & (2) & C13B-C14B & 1187 & (13) \\ O2-C41-O1 & 0.61 & (2) & C13B-C14B-H14B & 1258 \\ O2-C41-O1 & 54.45 & (18) \\ O2-C41-O1 & 0.61 & (2) & C13B-C14B-H14B & 1258 \\ O2-C41-O3Bii & 19.1 & (3) & O1B-C24B-C21B & 118.7 & (14) \\ O2-C41-O1 & 0.61 & (2) & C13B-C14B-H14B & 1258 \\ O2-C41-O3Bii & 19.1 & (3) & O1B-C24B-C21B & 118.7 & (13) \\ O2-C41-O3Bii & 19.1 & (3) & O1B-C24B-C21B & 118.7 & (13) \\ O2-C41-O3Bii & 19.1 & (3) & O1B-C24B-C21B & 118.7 & (14) \\ O1-C41-O3Bii & 19.3 & (3) & C1B-C2B-H20B & 119.9 \\ O1-C41-O3Bii & 19.5 & (3) & C1B-C2B-H$		1.508	())	C10A - C20A	1.30	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12—C11	1.450	(12)	C22A—H22A	0.930	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C12—C17Bix	1.462	(19)	C22A—C23A	1.35	(4)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C12—C17Aix	1.27	(4)	C15A—H15A	0.930	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C10 H10	0.020		C15A C16A	1.40	(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1.260	(12)		1.70	(0)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C10—C11	1.362	(13)	UI/A—UI8A	1.51	(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C10—C9	1.426	(13)	C17A—C16A	1.41	(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—H11	0.930		C23A—H23A	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{9}$ $C_{8}$	1 380	(11)	$C^{23}\Lambda = C^{18}\Lambda$	1 38	(4)
C8=C13A         L28         (2)         C20A-H20A         939           C8=C13A         1.64         (4)         C3B-H3B         0.930           C8=C5B         1.496         (9)         C3B-C3B         1.390           C1=C2A         1.517         (9)         C2B-C7B         1.390           C1=C2A         1.45         (3)         C7B-H7B         0.930           O3B-C24B         1.248         (12)         C7B-C6B         1.390           O2B-C16B         1.27         (4)         C6B-C5B         1.390           C16B-C17B         1.47         (2)         C4B-H4B         0.930           C16B-C17B         1.37         (2)         C5A-C4A         1.390           C19B-H19B         0.930         C5A-C4A         1.390         C19B-H19B         0.930           C19B-C18B         1.376         (18)         C6A-H6A         0.930         C13B-H18         0.930           C18B-C18B         1.322         (3)         C7A-H7A         0.930         C2A-C3A         1.390           C18B-H19B         0.930         C7A-H7A         0.930         C23B-C12B         1.390         C23B-C12B         1.390           C18B-C14B         1.322	C9-C8	1.380		C23A—C18A	1.30	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8-C13B	1.28	(2)	C20A—H20A	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8—C13A	1.64	(4)	C3B—H3B	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8-C5B	1 496	(9)	C3B—C2B	1 390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8 C5A	1.59	(2)	$C^{2}P$ $C^{4}P$	1 200	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Co-CJA	1.56	(3)	CJD—C4D	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C2B	1.517	(9)	C2B—C/B	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C2A	1.45	(3)	C7B—H7B	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O4B-C24B	1.248	(12)	C7B—C6B	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$O^2 P$ $C^2 4 P$	1 225	(14)	CAD HAD	0.020	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	03D	1.223	(14)		0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2BC16B	1.27	(4)	C6B—C5B	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2B-C13B	1.43	(3)	C5B—C4B	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C16B—C15B	1 47	(2)	C4B—H4B	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C16P C17P	1.27	(-)	C5A $C6A$	1 200	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Clob—Cl/B	1.37	(2)	CJA-COA	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19B—H19B	0.930		C5A—C4A	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19B—C18B	1.376	(18)	C6A—H6A	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19B—C20B	1 339	(19)	C6A—C7A	1 390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15P U15P	0.020	(1))		0.020	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0.950			0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15B—C14B	1.32	(3)	C/A—C2A	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C23B—H23B	0.930		C2A—C3A	1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C23B—C18B	1.32	(2)	СЗА—НЗА	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C^{22}P$ $C^{22}P$	1 20	$(\overline{2})$	$C_{2}^{2}$ $C_{4}^{A}$	1 200	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C25D-C22D	1.59	(2)		1.390	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	U21B-U24B	1.549	(19)	U4A—H4A	0.930	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21B—C22B	1.388	(18)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2-Cd1-O2i	153.1	(3)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02i—Cd1—O1i	54 45	(18)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$O_2 C_{41} O_1$	51 15	(10)	C22D C10D C10D	120.4	(15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		54.45	(18)	C25B-C18B-C19B	120.4	(15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2-Cd1-O11	106.1	(2)	C23B—C18B—C17B	121.3	(14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2i—Cd1—O1	106.1	(2)	C15B—C14B—C13B	108.3	(15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2i—Cd1—C1i	27 41	(19)	C15B—C14B—H14B	125.8	× /
02-cd1-c11 $151.8$ $(3)$ $C13B-c14B-H14B$ $125.8$ $02i-Cd1-O3Biii$ $119.1$ $(3)$ $04B-C24B-C21B$ $118.7$ $(13)$ $02-cd1-O3Biii$ $84.0$ $(3)$ $03B-C24B-O4B$ $125.2$ $(15)$ $02-cd1-O3Bii$ $119.1$ $(3)$ $03B-C24B-O21B$ $116.1$ $(11)$ $02i-Cd1-O3Bii$ $84.0$ $(3)$ $C23B-C22B-H22B$ $120.7$ $01i-Cd1-O1$ $98.3$ $(3)$ $C21B-C22B-H22B$ $120.7$ $01i-Cd1-O1$ $98.3$ $(3)$ $C21B-C22B-H22B$ $120.7$ $01-Cd1-C1i$ $27.15$ $(19)$ $C21B-C22B-H22B$ $120.7$ $01-Cd1-C1i$ $105.5$ $(3)$ $C19B-C20B-H22B$ $120.7$ $01-Cd1-O3Biii$ $96.2$ $(3)$ $C19B-C20B-H20B$ $119.9$ $01i-Cd1-O3Biii$ $96.2$ $(3)$ $C1B-C20B-H20B$ $119.9$ $01i-Cd1-O3Biii$ $96.2$ $(3)$ $C1B-C20B-H20B$ $119.9$ $01i-Cd1-O3Biii$ $96.2$ $(3)$ $C1B-C20B-H20B$ $119.9$ $01i-Cd1-O3Biii$ $96.2$ $(3)$ $C12ix-C17B-C18B$ $117.1$ $(13)$ $01-Cd1-O3Biii$ $165.3$ $(3)$ $C16B-C17B-C12ix$ $128.9$ $(17)$ $03Bii-Cd1-C1i$ $144.2$ $(3)$ $C16B-C17B-C18B$ $113.9$ $(16)$ $03Bii-Cd1-C1i$ $88.5$ $(3)$ $C24A-O3A-Cd2$ $138.2$ $(16)$ $03Bii-Cd1-O3Biii$ $69.3$ $(6)$ $C13A-N2A-C16A$ $96$ $(4)$	$O_2 C_{41} C_{11}$	121 0	(1)	C12D $C14D$ $U14D$	125.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02-cal-cll	131.8	(3)	C13B—C14B—H14B	123.8	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O21—Cd1—O3B111	119.1	(3)	O4B—C24B—C21B	118.7	(13)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—Cd1—O3Biii	84.0	(3)	O3B—C24B—O4B	125.2	(15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—Cd1—O3Bii	1191	(3)	O3B-C24B-C21B	116.1	(11)
O2I = Cd1 = O3Dii $O4.0$ $(3)$ $C23B = C22B = H22B$ $120.7$ $O1i = Cd1 = O1$ $98.3$ $(3)$ $C21B = C22B = C23B$ $118.7$ $(14)$ $O1i = Cd1 = C1i$ $27.15$ $(19)$ $C21B = C22B = H22B$ $120.7$ $O1 = Cd1 = C3Biii$ $96.2$ $(3)$ $C19B = C20B = H20B$ $120.1$ $O1 = Cd1 = O3Biii$ $96.2$ $(3)$ $C19B = C20B = H20B$ $119.9$ $O1i = Cd1 = O3Biii$ $165.3$ $(3)$ $C21B = C20B = H20B$ $119.9$ $O1i = Cd1 = O3Biii$ $96.2$ $(3)$ $C12Ix = C17B = C18B$ $117.1$ $(13)$ $O1 = Cd1 = O3Bii$ $165.3$ $(3)$ $C16B = C17B = C12ix$ $128.9$ $(17)$ $O3Bii = Cd1 = C1i$ $144.2$ $(3)$ $C16B = C17B = C18B$ $113.9$ $(16)$ $O3Bii = Cd1 = C1i$ $88.5$ $(3)$ $C24A = O3A = Cd2$ $138.2$ $(16)$ $O3Bii = Cd1 = O3Biii$ $69.3$ $(6)$ $C13A = N2A = C16A$ $96$ $(4)$	$O_{2i}$ $C_{d1}$ $O_{2}P_{ii}$	84.0	(3)	$C_{23B}$ $C_{23B}$ $U_{23B}$ $U_{23B}$	120.7	()
O11-Ca1-O198.3(3) $C21B-C22B-C23B$ 118.7(14) $O1i-Cd1-C1i$ 27.15(19) $C21B-C22B-H22B$ 120.7 $O1-Cd1-C1i$ 105.5(3) $C19B-C20B-C21B$ 120.1(12) $O1-Cd1-O3Biii$ 96.2(3) $C19B-C20B-H20B$ 119.9 $O1i-Cd1-O3Biii$ 165.3(3) $C21B-C20B-H20B$ 119.9 $O1i-Cd1-O3Biii$ 96.2(3) $C12ix-C17B-C18B$ 117.1 $O1-Cd1-O3Bii$ 96.2(3) $C16B-C17B-C12ix$ 128.9 $O1i-Cd1-O3Bii$ 165.3(3) $C16B-C17B-C12ix$ 128.9 $O1-Cd1-O3Bii$ 165.3(3) $C16B-C17B-C18B$ 113.9 $O3Bii-Cd1-C1i$ 144.2(3) $C16B-C17B-C18B$ 113.9 $O3Bii-Cd1-C1i$ 88.5(3) $C24A-O3A-Cd2$ 138.2 $O3Bii-Cd1-O3Biii$ 69.3(6) $C13A-N2A-C16A$ 96		04.0	(3)	$C_{23}D = C_{22}D = C_{22}D$	120.7	(1.4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	011-Ca1-01	98.3	(3)	C21B—C22B—C23B	118.7	(14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Oli—Cdl—Cli	27.15	(19)	C21B—C22B—H22B	120.7	
O1-Cd1-O3Biii96.2(3)C19B-C20B-H20B119.9O1i-Cd1-O3Biii165.3(3)C21B-C20B-H20B119.9O1i-Cd1-O3Biii96.2(3)C21B-C20B-H20B119.9O1i-Cd1-O3Bii96.2(3)C12ix-C17B-C18B117.1O1-Cd1-O3Bii165.3(3)C16B-C17B-C12ix128.9O3Biii-Cd1-C1i144.2(3)C16B-C17B-C18B113.9O3Bii-Cd1-C1i88.5(3)C24A-O3A-Cd2138.2O3Bii-Cd1-O3Biii69.3(6)C13A-N2A-C16A96	01—Cd1—C1i	105 5	(3)	C19B—C20B—C21B	120.1	(12)
$O_1$ —Cd1—O3Biii $90.2$ $(3)$ $C_{19B}$ —C20B—H20B $119.9$ $O1i$ —Cd1—O3Biii $165.3$ $(3)$ $C21B$ —C20B—H20B $119.9$ $O1i$ —Cd1—O3Bii $96.2$ $(3)$ $C12ix$ —C17B—C18B $117.1$ $(13)$ $O1$ —Cd1—O3Bii $165.3$ $(3)$ $C16B$ —C17B—C12ix $128.9$ $(17)$ $O3Biii$ —Cd1—C1i $144.2$ $(3)$ $C16B$ —C17B—C18B $113.9$ $(16)$ $O3Bii$ —Cd1—C1i $88.5$ $(3)$ $C24A$ —O3A—Cd2 $138.2$ $(16)$ $O3Bii$ —Cd1—O3Biii $69.3$ $(6)$ $C13A$ —N2A—C16A $96$ $(4)$		06 2	(3)	C10D $C20D$ $U20D$	110.0	(12)
O11-Cd1-O3Bin $165.3$ $(3)$ $C21B-C20B-H20B$ $119.9$ $O1i-Cd1-O3Bii$ $96.2$ $(3)$ $C12ix-C17B-C18B$ $117.1$ $(13)$ $O1-Cd1-O3Bii$ $165.3$ $(3)$ $C16B-C17B-C12ix$ $128.9$ $(17)$ $O3Biii-Cd1-C1i$ $144.2$ $(3)$ $C16B-C17B-C18B$ $113.9$ $(16)$ $O3Bii-Cd1-C1i$ $88.5$ $(3)$ $C24A-O3A-Cd2$ $138.2$ $(16)$ $O3Bii-Cd1-O3Biii$ $69.3$ $(6)$ $C13A-N2A-C16A$ $96$ $(4)$		90.Z	(3)		119.9	
Oli—Cd1—O3Bii         96.2         (3)         Cl2ix—Cl7B—Cl8B         117.1         (13)           Ol—Cd1—O3Bii         165.3         (3)         Cl6B—Cl7B—Cl2ix         128.9         (17)           O3Biii—Cd1—Cli         144.2         (3)         Cl6B—Cl7B—Cl8B         113.9         (16)           O3Bii—Cd1—Cli         88.5         (3)         C24A—O3A—Cd2         138.2         (16)           O3Bii—Cd1—O3Biii         69.3         (6)         Cl3A—N2A—Cl6A         96         (4)	011-Cd1-03B11	165.3	(3)	C21B—C20B—H20B	119.9	
O1Cd1O3Bii       165.3       (3)       C16BC17BC12ix       128.9       (17)         O3BiiiCd1C1i       144.2       (3)       C16BC17BC18B       113.9       (16)         O3BiiCd1C1i       88.5       (3)       C24AO3ACd2       138.2       (16)         O3BiiCd1O3Biii       69.3       (6)       C13AN2AC16A       96       (4)	O1i—Cd1—O3Bii	96.2	(3)	C12ix—C17B—C18B	117.1	(13)
O3Biii-Cd1-Cli144.2(3)C16B-C17B-C18B113.9(16)O3Bii-Cd1-Cli $88.5$ (3)C24A-O3A-Cd2 $138.2$ (16)O3Bii-Cd1-O3Biii $69.3$ (6)C13A-N2A-C16A $96$ (4)	O1—Cd1—O3Bii	165 3	(3)	C16B—C17B—C12ix	128.9	(17)
O3Bii-Cd1-C1i $144.2$ $(3)$ $C10B-C1/B-C18B$ $113.9$ $(16)$ $O3Bii-Cd1-O3Biii$ $88.5$ $(3)$ $C24A-O3A-Cd2$ $138.2$ $(16)$ $O3Bii-Cd1-O3Biii$ $69.3$ $(6)$ $C13A-N2A-C16A$ $96$ $(4)$	$O2P_{iii}$ $Cd1$ $C1i$	144 0	(3)	C16D C17D C12IX	1120	(16)
U3BII $U11$ <		144.2	(3)		113.7	(10)
O3Bii—Cd1—O3Biii 69.3 (6) C13A—N2A—C16A 96 (4)	O3Bii—Cd1—Cli	88.5	(3)	C24A—O3A—Cd2	138.2	(16)
	O3Bii—Cd1—O3Biii	69.3	(6)	C13A—N2A—C16A	96	(4)

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	044	112.0		N24 C124 C0	112	(5)
$\begin{array}{c} 0.464 = -0.11 & -0.16 & -0.150.88 & -0.15 & -0.16 & -0.150.88 & -0.15 & -0.16 & -0.15 - 0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.15 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & -0.16 & $	04A11 - Ca1 - 02	113.9	(6)	N2A = C13A = C8	113	(5)
$\begin{array}{c} \begin{array}{c} \begin{array}{c} 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0$	04Aii - Cd1 - 01	02.2 166 5	(0)	$\frac{112A}{C14A} = C13A = C14A$	122	(3)
$\begin{array}{c} \mbox{Cd2} - 0.7 & \mbox{S1} + \mbox{S2} & \mbox{S3} + \mbox{S3} + \mbox{S3} + \mbox{S3} + \mbox{S4} + \mbox{S3} + \mbox{S4} + \mbo$	O4Aiii = Cd1 = O1	77.6	(0)	$C_{14A} = C_{15A} = C_{8}$	123	(4) (2)
$ \begin{array}{c} \label{eq:constraints} \begin{array}{c} \mbox{constraints} \\ constrain$	$O_{2}iv - Cd^2 - O_{2}v$	81.4	(3)	C20A - C21A - C24A	117	(2)
$ \begin{array}{c} \label{eq:constraints} \begin{array}{c} \mbox{CD} = -0.2 \mbo$	O2v—Cd2—O3Aviji	155.2	(6)	C20A - C21A - C24A	123	(2)
$\begin{array}{c} 020 & -022 & -03A & 023 & 023 & 023 & 023 & 023 & 023 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024 & 024$	$O_2 v = Cd_2 = O_3 A v m$	155.2	(6)	$C_{20A} = C_{21A} = C_{24A}$	127.8	(2)
$\begin{array}{c} c_{D} - c_{D} -$	$O_{2iv} = Cd_2 = O_{3A}$	78.2	(0)	C13A = C14A = III4A	127.0	(4)
$ \begin{array}{c} \operatorname{Cd}} \operatorname{Cd}_{2} & C$	$O_{2V} = Cd_2 = O_{3A}$	78.2	(5)	C15A - C14A - C15A	104	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$O_2 v = Cd_2 = O_3 A$	106.2	(3)	C13A - C14A - II14A	127.0	
$ \begin{array}{c} \operatorname{cd} \operatorname{cd} = -\operatorname{cd} = -\operatorname{cd} & \operatorname{cd} & $	O4Bvii = Cd2 = O2iv	76.8	$\binom{2}{3}$	$C_{10A} = C_{10A} = H_{10A}$	110.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O4Bvii = Cd2 = O2iv	76.8	(3)	$C_{20A} = C_{19A} = \Pi_{19A}$	110.0	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O4Bvii = Cd2 = O2v	106.2	(3)	$C_{20}A - C_{13}A - C_{18}A$	122	(3)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	O4Bvii = Cd2 = O2v	176.2	$\binom{2}{4}$	$C_{21A} = C_{22A} = \Pi_{22A}$	120.0	(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	O4Bvi = Cd2 = O4Bvii	05.5	(4)	$C_{23A} = C_{22A} = C_{21A}$	120.8	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O4Bvii = Cd2 = O3Aviii	828	(5)	$C_{23}A - C_{22}A - H_{12}A$	126.8	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$O_3 A_{\text{viii}} = Cd_2 = O_3 A_{\text{viii}}$	124.8	(3) (11)	$C_{14A} = C_{15A} = C_{14A}$	120.0	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cd1 = O2 = Cd2iii	105 7	(11) (2)	C16A - C15A - C14A	126.8	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1 = O2 = Cd1	02.5	(2)	C10A - C13A - C18A	120.8	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1 = O2 = Cd1 C1 = O2 = Cd2iii	149.9	(4)	C12ix— $C17A$ — $C16A$	117	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C1 = O2 = Cd2III	02 /	(5)	$C12I_{A}$ $C17A$ $C18A$	122	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C12_N1_H1$	92. <del>4</del> 125 7	$(\mathbf{J})$	$C_{10A} = C_{1/A} = C_{10A}$	116.2	(ד)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C12_N1_C9$	123.7	(7)	$C_{22A} = C_{23A} = C_{18A}$	178	(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	100.7	(I)	$C_{22A} = C_{23A} = C_{10A}$	116 2	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1_C12_C11	123.7	(7)	C10A - C23A - H23A $C10A - C18A - C17A$	123	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N1 - C12 - C11 N1 - C12 - C17 Biv	100.4	(1)	$C_{13A} = C_{10A} = C_{10A}$	123	(3)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C11\_C12\_C17Biv$	123.2	(10) (11)	$C_{23} = C_{10} = C_{17} = C$	173	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C17 Aix C12  C12  N1	120.1	(11) (18)	$C_{23}$ $C_{16}$ $C$	123	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C17Aix = C12 = C11	1163	(18) (17)	C15A - C16A - C17A	122	(4)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C11 - C10 - H10	126.1	(17)	C17A = C16A = C17A	122	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_{11} = C_{10} = C_{10}$	120.1	(8)	O1/A = C10A = N2A	128	(4) (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C1 - C10 - C3	107.0	(8)	O4A = C24A = O3A	120	(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_{12}$ $C_{11}$ $H_{11}$	120.1		04A - C24A - C21A	115	(2) (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_{12}$ $C_{11}$ $C_{12}$ $C_{11}$ $C_{12}$	120.7	(0)	$C_{21A} = C_{24A} = C_{21A}$	110.6	(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C10 - C11 - U12	100.0	(9)	$C_{21A} = C_{20A} = H_{20A}$	119.0	(2)
$\begin{split} &  A  = -5 - C_{10} &  108.3 \\ C B  = -120A \\ C$	C10-C11-H11	120.7	(9)	C19A - C20A - C21A	121	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1 - C9 - C10	108.5	$\begin{pmatrix} 8 \end{pmatrix}$	C19A - C20A - H20A	119.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	NI = C9 = C8	120.0	$(\delta)$	C2B = C3B = C4B	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{0} = C_{0} = C_{10}$	124.8	$\binom{7}{2}$	$C_{2B}$ $C_{3B}$ $C_{4B}$ $C_{4B}$ $C_{2B}$ $H_{2B}$	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9 = C8 = C13A	124	$\binom{2}{0}$	C4B - C3B - H3B	120.0	(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{2}$	120.2	(9)	C3B = C2B = C1	118.0	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{12} = C_{2} = C_{2}$	109.2	(18)	C/B = C2B = C1	121.8	(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C13B - C3 - C9	120.2	(12)	C/B = C2B = C3B	120.0	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	02-C1-C2B	120.8	(0)	$C_{2B}$ $C_{7B}$ $C_{6B}$	120.0	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	02-C1-C2A	113.8	(10) (7)	$C_{2B}$ $C_{7B}$ $U_{7B}$	120.0	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	01 - C1 - 02	120.2	(7)	COB - C/B - H/B	120.0	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	OI = CI = C2B	119.0	(/) (15)	C/B = C0B = H0B	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	OI = CI = C2A	123.0	(13)	$C_{B} = C_{B} = C_{B}$	120.0	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C_{24}D = C_{4}D = C_{4}L_{2}$	137.0	(0) (0)		120.0	(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{4B} = C_{3B} = C_{4B}$	98.4 112 2	(9)	CAD - CAD - CAD	121.8	(0)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	U10B - IN2B - U15B	113.2	(17) (10)	C4B = C5B = C4B	120.0	(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2D = C16D = C17D	100.0	(19)	$C4D - C3D - C\delta$	118.1	(0)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2D - U10B - U1/B	125	(2) (2)	$C_{2}B - C_{4}B - H_{4}B$	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19D C10B U10D	129	(2)	C5D C4D U4D	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{10}B = C_{10}B = H_{10}B$	119./			120.0	( <b>2</b> )
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C20B C10B C10B	119.7	(14)	CA - CA - CA	11/	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{7}$	120.7	(14)	CA - CA - CA	120.0	( <b>2</b> )
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CIAD CIED CIED	125.4	(10)	$C_{4A}$ $C_{5A}$ $C_{6A}$ $U_{6A}$	125	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C14B = C15B = C16B	109.2	(18)	$C_{A} = C_{A} = C_{A}$	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{14B} = C_{12B} = H_{12B}$	125.4		C/A = COA = COA	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{10}B = C_{20}B = C_{20}B$	119.2	(14)	C/A = COA = HOA	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{22}D = C_{22}D = U_{22}D$	121./	(14)	COA - C/A - H/A	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{22}B = C_{23}B = H_{23}B$	119.2	(12)	$C_{A}$ $C_{A}$ $C_{A}$ $C_{A}$	120.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C22B—C21B—C24B	120.5	(13)	$C_{A}$ $C_{A}$ $H_{A}$	120.0	
C20BC21BC24B       121.3       (11)       C7AC2AC3A       120.0         C8C13BN2B       132       (2)       C3AC2AC1       124       (2)         C8C13BC14B       125.2       (17)       C2AC3AH3A       120.0         N2BC13BC14B       103.1       (18)       C4AC3AC2A       120.0         C19BC18BC17B       118.2       (14)       C4AC3AH3A       120.0         C3AC4AH4A       120.0       C3AC4AC5A       120.0	C22B—C21B—C20B	118.2	(13)	C/A - C2A - C1	116	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C20B—C21B—C24B	121.3	(11)	C/A—C2A—C3A	120.0	
C8—C13B—C14B       125.2       (17)       C2A—C3A—H3A       120.0         N2B—C13B—C14B       103.1       (18)       C4A—C3A—C2A       120.0         C19B—C18B—C17B       118.2       (14)       C4A—C3A—H3A       120.0         C5A—C4A—H4A       120.0         C3A—C4A—C5A       120.0	C8—C13B—N2B	132	(2)	$C_3A - C_2A - C_1$	124	(2)
N2B-C13B-C14B         103.1         (18)         C4A-C3A-C2A         120.0           C19B-C18B-C17B         118.2         (14)         C4A-C3A-H3A         120.0           C5A-C4A-H4A         120.0           C3A-C4A-C5A         120.0	C8—C13B—C14B	125.2	(17)	С2А—СЗА—НЗА	120.0	
C19B—C18B—C17B 118.2 (14) C4A—C3A—H3A 120.0 C5A—C4A—H4A 120.0 C3A—C4A—C5A 120.0	N2B-C13B-C14B	103.1	(18)	C4A—C3A—C2A	120.0	
C5A—C4A—H4A 120.0 C3A—C4A—C5A 120.0	C19B—C18B—C17B	118.2	(14)	С4А—СЗА—НЗА	120.0	
<u>C3AC4AC5A</u> 120.0				CSA—C4A—H4A	120.0	
				C3A—C4A—C5A	120.0	

 $\begin{array}{c} \hline C3A-C4A-H4A & 120.0 \\ \hline Symmetry codes: (i) -x+3, y, -z+3/2; (ii) -x+3/2, y+1/2, -z+3/2; (iii) x+3/2, y+1/2, z; (iv) -x+1/2, y-1/2, -z+3/2; \\ (v) x-3/2, y-1/2, z; (vi) -x, y, -z+3/2; (vii) x-1, y, z; (viii) -x-1, y, -z+3/2; (ix) -x+1/2, -y+3/2, -z+1; (x) x+1, y, z. \end{array}$ 

#### Topology analysis of compound 1

The topology of compound **1** was performed with the ToposPro program package and the TTD collection of periodic network topologies.<sup>1</sup> If we carry out simplification by standard procedure, we obtain a 4,4,8-c net, which is a new trinodal network (Fig. S1(d)). It will be named *nnu3* and will be added to TTD-collection in the following update. The point symbol of the net is  $(4^4.6^2)_2(4^8.6^4.8^{16})$ . Both types of 4-coordinated nodes correspond to Cd atoms (Fig. S1(a) and Fig. S1(b)), the 8-coordinated nodes are the centers of mass of 5,10,15,20-*tetrakis*(4-carboxylatophenyl) porphyrin) ligands (Fig. S1(c)).



#### Fig. S1 4,4,8-c underlying net (nnu3) of compound 1.

(a) the coordination mode of one sort of Cd atoms.(b) the coordination mode of second sort of Cd atoms. (c) the O<sup>44</sup> coordination mode of a 5,10,15,20-*tetrakis*(4-Carboxylatophenyl)porphyrin) ligand. (d) the overall net.

Another method of analysis of compound 1 is the cluster simplification procedure. Compound 1 contains one-periodic secondary building units, they are called rod SBUs (Fig. S2(a))<sup>2</sup> The composition of infinite rod is  $[CdC_2O_4]_n$ . The Cd atoms form two types of polyhedra: trigonotritetrahedron (8 O atoms) and tetrahedron (4 O atoms), which share the opposite edges (Fig.S2(b)). Each rod SBU is connected to eight other rods by four ligands as shown in Fig. S2(c). If we project atoms on the (100) plane (Fig. S2(c), we can conclude, that there are two kinds of nonequivalent 4-coordinated nodes: the projections of the middle lines of the rods and the centers of the mass of the ligands. As a result, structure has tetragonal rod packing.



#### Fig. S2 The rod packing structure of compound 1

(a) the parallel rod SBUs, (b) the projection of parallel rod SBUs on the (100) plane, (c) the  $[CdC_2O_4]_n$  rod constructed by edge-sharing polyhedra.

Compound 1 can be simplified in a third way by the cluster simplification method. This method proposes to consider some valence bonds, in particular, C1-C2, C5-C8, C13-C14 and C17-C20 as intercluster (Fig. S3(a)). Additionally, we manually changed all valence bonds of Cd2 atoms to intercluster for isolation of the  $CdC_4O_8$  clusters, which contain only Cd1 atoms (Fig. S3(b)). Now, there are no parallel infinite valence bonded  $CdC_2O_4$  clusters and we can provide the second step of the classical cluster simplification procedure: all valence-bonded groups should be contracted to their centers of mass. The resulting underlying net is 2-nodal 4,6-coordinated with point symbol  $(4^2.6^4)(4^2.6^8.7^3.8^2)$ . Topological type is 4,6T156. The coordination modes of the central atoms, ligands and the underlying net itself are showed in Fig. S3(c)-(f)).



#### Fig. S3 The 2-nodal 4,6-coordinated 4,6T156 topology of compound 1.

(a) 5,10,15,20-*tetrakis*(4-Carboxylatophenyl)porphyrin) ligand after cluster simplification. (b) Separated clusters with the composition CdC<sub>4</sub>O<sub>8</sub> (Cd1) by Cd2 atoms. (c) The coordination mode of a 5,10,15,20-*tetrakis*(4-carboxylatophenyl)porphyrin) ligand. Black balls is the center of mass of the ligand; magenta balls are centers of mass of the CdC<sub>4</sub>O<sub>8</sub> clusters (they coincide with Cd atoms). (d) the coordination mode of a Cd1 atom. (e) 4,6T156 net (f) the initial structure and the 4,6T156 net are combined.

The TTD collection contains only five records for 4,6T156 topological type. There is an isostructural series of four compounds, which are constructed by the same ligand (5,10,15,20-*tetrakis*(4-carboxylatophenyl)porphyrin)),<sup>3</sup> the fifth compound contains a  $\mu$ -4,4',4",4"'-pyrene-1,3,6,8-tetrayltetrabenzoate ligand.<sup>4</sup>

#### **IR** spectra

We recorded the IR spectrum of  $H_6TCPP$ , which is consistent with the reported spectrum.<sup>5</sup> We also recorded the Raman spectrum of  $H_6TCPP$  (Fig. S4(c)). The IR spectra of **1-DMF**, **1(4:1)-4d-DMF**, **1(6:1)-4d-DMF** and **1(8:1)-4d-DMF** (Fig. S4(a)) are all the same, showing a band at 1707 cm<sup>-1</sup> which is too high to be assigned to a C=O stretching of DMF molecules (1670-1690 cm<sup>-1</sup>). By comparing the IR spectrum of **1(8:1)-4d-DMF** with those of **1-ex** and  $H_6TCPP$  in Fig. S4(c), we think this band is due to  $H_6TCPP$  trapped between crystals or in the channels, which was not washed completely away by DMF solvent. In contrast, the solvent exchanged sample (**1-ex**) contains no  $H_6TCPP$  and DMF molecules and should represent the IR spectrum of compound **1**. The IR peaks of  $H_6TCPP$  at 3420, 1695, 1405, and 1265 cm<sup>-1</sup> (Fig. S4(c)) are assigned to the stretching vibrations of O-H, C=O, and C-O bonds of carboxylic acid groups according to literature.<sup>5-7</sup> Consistently, the Raman spectrum of  $H_6TCPP$  (Fig. S4(c)) shows no strong peaks in the range of those frequencies since these bonds are all very polar. The strong band at 1605 and the weak peak at 1560 cm<sup>-1</sup> were assigned by others to C=C and C=N stretchings.<sup>5-7</sup> The C=O distances are varied in a relatively large range according to the crystal structure of **1** (e.g. 1.2500(74), 1.26(2) and 1.29(2) Å in **1**). Thus it is possible there are two bands due to asymmetric stretching of CO<sub>2</sub><sup>-</sup>. Since 1541 cm<sup>-1</sup> is very strong, it should not be a C=C stretching band, we therefore assigned the strong bands at 1603 and 1541 cm<sup>-1</sup> to asymmetric stretching of CO<sub>2</sub><sup>-</sup>.



Fig. S4 IR spectra of 1-DMF, 1-ex, 1(4:1)-4d-DMF, 1(6:1)-4d-DMF, and 1(8:1)-4d-DMF (a); IR spectra of Li<sup>+</sup>-1-2d, Li<sup>+</sup>-1-5d, and Li<sup>+</sup>-1-10d (b); IR and Raman spectra of H<sub>6</sub>TCPP compared with IR spectra of 1-ex and 1(8:1)-4d-DMF (c).







Fig. S5 TG (blue)/DTA(red)/DTG(green) of MOF 1 and its derived products.



Fig. S6 PXRD spectrum of 1-DMF after two cycles of photocatalytic CO<sub>2</sub> reduction.



Fig. S7 CO<sub>2</sub> (273 and 298 K) and CH<sub>4</sub> (273 and 298 K) adsorption/desorption isotherms of 1(4:1)-4d-ex (a), 1(6:1)-4d-ex (b), and 1(8:1)-4d-ex (c).



Fig. S8 CO<sub>2</sub> (273 and 298 K) and CH<sub>4</sub> (273 and 298 K) adsorption/desorption isotherms of Li<sup>+</sup>-1-5d (a) and Li<sup>+</sup>-1-10d (b).



Fig. S9 Band gaps of 1(4:1)-4d-ex, 1(6:1)-4d-ex, 1(8:1)-4d-ex, Li<sup>+</sup>-1-2d, Li<sup>+</sup>-1-5d, and Li<sup>+</sup>-1-10d determined by plots of (*abs* or [*abs*(hv)]<sup>1/2</sup> or [*abs*(hv)]<sup>2</sup> versus hv.



**Fig. S10** Cathodic and anodic linear potential scans for determining the positions of the CB and VB edges of 1-DMF, and 1-ex using  $pH=5.34 H_2SO_4$  aqueous solution or the **Tris-HCI buffered saline solution (0.1 mol L**<sup>-1</sup>, **pH 7.4**)). The red curves are the currents of the electrolytes using the unmodified ITO electrodes.



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Fig. S11 Cathodic and anodic linear potential scans for determining the positions of the CB and VB edges of 1(4:1)-4d-ex ((a)-(d)), 1(6:1)-4d-ex ((e)-(h)) and 1(8:1)-4d-ex ((i)-(l)) using two different electrolytes (the pH 5.01 H<sub>2</sub>SO<sub>4</sub> aqueous solution or the Tris-HCl buffered saline solution (0.1 mol·L-1, pH 7.4)). The red curves are the currents of the electrolytes using the unmodified ITO electrodes.

![](_page_17_Figure_0.jpeg)

![](_page_18_Figure_0.jpeg)

**Fig. S12** Cathodic and anodic linear potential scans for determining the positions of the CB and VB edges of Li<sup>+</sup>-1-2d ((a)-(d)), Li<sup>+</sup>-1-5d ((e)-(h)) and Li<sup>+</sup>-1-10d ((i)-(l)) using two different electrolytes (the pH 5.01  $H_2SO_4$  aqueous solution or the **Tris-HCI buffered saline solution (0.1 mol L**<sup>-1</sup>, pH 7.4)). The red curves are the currents of the electrolytes using the unmodified ITO electrodes.

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